

# Single-cluster algorithm for the site-bond-correlated Ising model

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## Abstract

We extend the Wolff algorithm to include correlated spin interactions in magnetic systems. This algorithm is applied to study the site-bond-correlated Ising model on a two dimensional square lattice. We use a finite size scaling procedure to obtain the phase diagram in the temperature-concentration  $(T_c, C)$  space.

PACS numbers: 05.50.+q; 64.60.-i; 75.40Mg

For randomly diluted magnetic systems the critical concentration where the magnetic order vanishes is of great interest. The dependence of the critical temperature with the concentration is ruled by the topological properties of the lattice and by the symmetry of the interaction Hamiltonian.

In the simplest description of a dilute magnet, the occupied lattice sites correspond to the magnetic atoms and the empty sites are associated with the presence of nonmagnetic atoms (impurities). Interactions are short ranged usually of the exchange interaction type. The strength of the exchange interaction is not affected by their neighbors. At  $T = 0$ , the cluster structure is well described by the ordinary site percolation model.

However, it has been found experimentally that sometimes the *local environment* may modify the exchange coupling constant between two atoms or may even suppress their magnetic manifestations. This means that interactions involving more than two atoms are present in the system. To take these effects into account, two kinds of correlations were proposed: the long and the short ranged correlation models. The bootstrap percolation model [1] is a good example for the former and the site-bond-correlated model [2, 3] for the latter. Long-ranged correlation may change the critical exponents or even the order of the transition of its corresponding uncorrelated model. In contrast, the short-ranged correlation seems to be unable to such drastic effects. Anyway, for these systems, dilution as well as correlation play an important role.

An analysis of  $^{19}\text{F}$  NMR linewidths in the randomly diluted magnetic

system  $KNi_xMg_{1-x}F_3$  and in the isostructural compound  $KMn_xMg_{1-x}F_3$  ( where  $x$  is the concentration ) show remarkable differences in their properties [2, 4]. For instance, the concentration or percolation threshold where the magnetic order ceases are different. Further, the former displays an upward curvature in the temperature-concentration plane which is absent in the latter. In order to explain these facts, Aguiar *et al.* [2] proposed a dilution model where the exchange coupling constant of two ions  $Ni^{2+}$  depends directionally on the magnetic attributes of their nearest neighbor atoms. That is the magnetic spins are correlated. In a subsequent work [3], a parameter  $\alpha$  was introduced which is a measure of the correlation strength. When  $\alpha > 0$  or  $\alpha < 0$  we have *ferro* or *antiferromagnetic correlation*, respectively. Due to the presence of both ferro and antiferromagnetic coupling constants, the antiferromagnetic correlation brings competition to the system and a spin glass behavior is expected.

The thermal properties of the site-bond-correlated Ising model (hereafter denoted SBC) was investigated using several approaches: mean field [3], Honmura-Kaneyoshi effective-field [5], renormalization group [6, 7] and Monte Carlo renormalization group [8]. Any of these techniques lead to almost the same physical scenario with the exception of the SBC defined on the Bethe lattice [9]. Here there are some unexpected features which seem to be due to the pathological geometry of the Bethe lattice. Also the SBC cluster characteristics has been studied and its connection with the percolation problem. For the square lattice, it is now well established that there are two kinds of percolations: the usual site

percolation with threshold  $p_c \sim 0.592$  when  $0 < \alpha \leq 1$  and a *correlated* percolation with threshold  $p_c \sim 0.740$  at  $\alpha = 0$  [10]. There are now strong indications that both percolations belong to the same universality class [11, 12].

As far as we know, reference [13] is the only work which treats the thermal properties of the SBC model by using the Monte Carlo technique. In that paper, the parameter  $\alpha$  is restricted to be null. Everyone knows that is very difficult to simulate near phase transitions due to the emergence of the critical slowing down phenomenon. In the SBC this becomes even worst since dilution together with correlation conspire to weaken the Metropolis technique. Fortunately, for the so called *cluster algorithms* the dilution turns these algorithms even more robust [14]. In the Ising model (diluted or not) the Metropolis algorithm is a local Monte Carlo method where only one spin is flipped each time. For the *cluster algorithms* however, the entire cluster can be flipped. Indeed, there are actually two kinds of cluster algorithms: the single-cluster algorithm like the Wolff [15] algorithm and those involving multiple clusters as the Swendsen-Wang [16] and the invaded cluster [17] algorithms. In this paper we generalize the Wolff algorithm to include correlation. We use our results to construct the SBC phase diagram for many concentrations and for the correlation  $\alpha$  in the interval  $[0, 1]$ .

In spite of the great interest received during the last decades by the critical slowing down phenomenon, it is still a hard question to find under what conditions it can be reduced. Two independent strand of thought had contribute

to enlighten the problem. The first was the search for the so called "physical cluster" of the Ising model. The idea is to find a percolation problem in absolute harmony with the thermal problem: the temperature where the percolation threshold occurs ( $T_p$ ) must coincide with the critical temperature ( $T_c$ ) and also their corresponding critical exponents need to be the same. The "geometrical cluster", i. e., those clusters formed by grouping all nearest neighbors up (or down) spins were discarded since in 3-d they neither have  $T_p = T_c$  nor are their exponents the same. The first explicit construction of "physical clusters" was proposed by Coniglio and Klein [18]. Parallel to this research line, Fortuin and Kasteleyn [19] introduced the random cluster model. They proved that the susceptibility of the Ising model is equal to the mean cluster size of the random cluster model. Gathering these ideas, Swendsen and Wang [16] developed a new algorithm for the Potts model. In this algorithm, clusters of spins in the same states are grown and flipped. Thus, a number of spins are update in a single move and the correlation time is reduced.

In 1989, a *single-cluster* Monte Carlo algorithm was introduced by Wolff [15] for the  $O(N)$  spin models as a variation on the Swendsen-Wang scheme for the Ising model and has proved to be even more effective. In the Wolff algorithm only one cluster is formed and flipped with probability 1, whereas in the Swendsen-Wang dynamics all percolation clusters are formed and flipped with probability 1/2. According to Tamayo et al. [20] the main reason for a better performance of the Wolff algorithm is that the mean size of the clusters

flipped is significantly larger than in Swendsen-Wang case.

In the SBC model the presence of nonmagnetic impurities in the neighborhood of a given pair of nearest-neighbor magnetic atoms can modify the strength of the exchange interaction between the two atoms. Moreover, in the limit of strong correlation  $\alpha$ , the correlation can even suppress the relevant exchange interaction.

The model Hamiltonian is the following

$$H = - \sum_{i,\delta} J_{i,i+\delta} (\sigma_i \sigma_{i+\delta} - 1) \quad (1)$$

where  $\sigma_i = \pm 1$  and  $\delta$  denotes an elementary lattice vector. The exchange interaction  $J_{i,i+\delta}$  is given by

$$J_{i,i+\delta} = J \varepsilon_i \varepsilon_{i+\delta} [(1 - \alpha) \varepsilon_{i-\delta} \varepsilon_{i+2\delta} + \alpha], \quad (2)$$

where  $J > 0$ . The random variables  $\varepsilon_i$  can take values one with probability  $C$  and zero with probability  $1 - C$ , where  $C$  is the concentration of magnetic atoms. The parameter  $\alpha$  correlates the interaction between sites  $i$  and  $i + \delta$  with the magnetic occupancy of the sites  $i - \delta$  and  $i + 2\delta$ . The uncorrelated dilute Ising model is re-obtained in the limit  $\alpha = 1$ . For  $0 < \alpha < 1$ , the bond between  $i$  and  $i + \delta$  is only weakened by the absence of a magnetic atom at  $i - \delta$  or  $i + 2\delta$ . The limit  $\alpha = 0$  corresponds to the maximum correlation, i. e., two magnetic first neighbor sites are connected by an active bond only if their nearest-neighbor sites along the line joining them are also present.

In the Wolff algorithm for the pure Ising model, first a site is randomly chosen in the lattice. A nearest neighbour site will be added to the cluster with an activation probability  $p = 1 - e^{-2K}$  (where  $K = \frac{J}{K_B T}$ ) if it is in the same spin state. This procedure is repeated until no more sites can be incorporated to the cluster. The whole cluster is then flipped. Following Fortuin-Kasteleyn [19], we derive the bond activation probability:

$$\begin{cases} p_{i,i+\delta} = 0 & \text{if } \sigma_i \neq \sigma_{i+\delta} \\ p_{i,i+\delta} = 1 - e^{-2K} & \text{if } \sigma_i = \sigma_{i+\delta} \text{ and } \varepsilon_{i-\delta}\varepsilon_{i+2\delta} = 1 \\ p_{i,i+\delta} = 1 - e^{-2\alpha K} & \text{if } \sigma_i = \sigma_{i+\delta} \text{ and } \varepsilon_{i-\delta}\varepsilon_{i+2\delta} = 0 \end{cases}$$

between sites  $i$  and  $i + \delta$ . The definition of these activation probabilities guarantees correctly the applicability of the cluster dynamics and constitutes the Fortuin-Kasteleyn mapping for the SBC model.

We simulate the SBC model for various values of correlation ( $\alpha$ ) and concentration ( $C$ ) on a square lattice of size  $L = 50, 100, 150$  and  $300$ . A random uniformly distributed magnetic sites configuration (or simply *sample*) is generated with an occupation probability  $C$ . Over this quenched (geometric) configuration, an *initial* spin configuration is chosen with half of the spins up. One Wolff's cluster is then constructed using the activation probabilities just described. The entire cluster is then flipped and the new magnetization is determined. We call the sequence: cluster construction + flipping + magnetization measure *one* iteration or Monte Carlo step. Our first 1000 iterations were discarded waiting the system to achieve the thermal equilibrium. The remaining iterations were used to measure the mean magnetization and its fluctuation -

the magnetic susceptibility. On these quantities, another average over the samples was necessary in order to anneal the geometric influence (always present in diluted systems). Finally, we scan the coupling  $K$  to find  $K_{max}$  where the susceptibility is maximum. In Table 1 we show the number of iterations and realizations necessities to reduce the error of  $K_{max}$  to  $\sim 0.01$ . Of course, they depend on the values of  $\alpha$  and  $C$ .

Table 1 to be inserted

The determination of  $K_{max}$  was done for fixed values of  $\alpha$ ,  $C$  and  $L$  and then extrapolated to the thermodynamic limit  $L \rightarrow \infty$  through the BST algorithm [21]. The BST is a useful algorithm to extrapolate physical quantities that converge obeying a power law  $F(L) = F(L = \infty) + AL^{-\Theta}$ . It allows a reliable determination of critical parameters in the limit  $L \rightarrow \infty$  and its versatility becomes more pronounced if there are only very short sequences available.

Figure 1 to be inserted

The phase diagram is shown in Fig. 1. The initial slope  $(1/T_c)(dT_c/dC)$  at the pure  $C = 1$  case increases with the degree of correlation, which is supported by both experimental [2] and theoretical [3, 5, 13] data. At  $T = 0$ , we obtain two distinct percolation threshold: one for  $\alpha = 0$  and another for  $\alpha \neq 0$ . It can be seen in the figure that the curves for intermediate correlation  $0 < \alpha < 1$  have an upward curvature ( not present in extreme the cases  $\alpha = 0$  and  $\alpha = 1$ ) in agreement with the experimental results for the  $KNi_xMg_{1-x}F_3$  compound



[2]. In summary, we have generalized the Wolff's algorithm for systems where both dilution and correlation are present. This allowed us to get the phase diagram of the site-bond-correlated Ising model on a two dimensional square lattice. The natural question on how the new algorithm changes the dynamical critical exponent and the autocorrelation time is now under investigation.

We acknowledge Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Fundação de Amparo a Pesquisa do Estado de São Paulo (FAPESP) for financial support.

## References

- [1] J. Chalupa, P. L. Leath and G. R. Reich, J. Phys. C **12**, L31 (1979).
- [2] J. Albino O. de Aguiar, M. Engelsberg and H. J. Guggenheim, J. Magn. Mater. **54-57**, 107 (1986).
- [3] J. Albino O. de Aguiar, F. G. Brady Moreira and M. Engelsberg, Phys. Rev. B **33**, 652 (1986).
- [4] M. Engelsberg, J. Albino O. de Aguiar, O. F. de Alcantara Bonfim and A. Franco Jr., Phys. Rev. B **32**, 7143 (1985).
- [5] A. A. P. da Silva and F. G. B. Moreira, Phys. Rev. B **40**, 10986 (1989).
- [6] N. S. Branco, S. L. A. de Queiroz and R. R. dos Santos, Phys. Rev. B **38**, 946 (1988).
- [7] N. S. Branco, S. L. A. de Queiroz and R. R. dos Santos, Phys. Rev. B **42**, 458 (1990).
- [8] N. S. Branco and K. D. Machado, Phys. Rev. B **47**, 493 (1993).
- [9] S. Coutinho, J. A. O. de Aguiar, F. G. B. Moreira and J. R. L. de Almeida, Phys. Rev. B **36**, 8478 (1987).
- [10] O. F. A. Bonfim and M. Engelsberg, Phys. Rev. B **34**, 1977 (1986).
- [11] L. M. de Moura and R. R. dos Santos, Phys. Rev. B **45**, 1023 (1992).

- [12] P. R. A. Campos, L. F. C. Pessoa and F. G. B. Moreira, to be published  
in Phys. Rev. B.
- [13] A. J. F. de Souza and F. G. B. Moreira, J. Phys. (Paris) **49**, C8 (1988).
- [14] M. Hennecke and U. Heyken, J. Stat. Phys. **72**, 829 (1993).
- [15] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).
- [16] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. **58**, 86 (1987).
- [17] J. Machta, Y. S. Choi, A. Lucke and T. Schweizer, Phys. Rev. Lett. **75**,  
2792 (1995).
- [18] A. Coniglio and W. Klein, J. Phys. A **13**, 2775 (1980).
- [19] P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Japan **26** (Suppl.), 11  
(1969); C. M. Fortuin and P. W. Kasteleyn, Physica **57**, 536 (1972).
- [20] P. Tamayo, R. C. Brower and W. Klein, J. Stat. Phys. **58**, 1083 (1990).
- [21] R. Bulirsch and J. Stoer, Numer. Math. **6**, 413 (1964).

### Table Caption

**Table 1** - Range of the number of samples  $N_s$  and number of iterations  $N_i$  used in this work. The numbers  $N_s$  and  $N_i$  augment for smalls  $\alpha$  (strong correlation) and  $C$  (strong dilution).

### Figure Caption

**Fig. 1** - The SBC Ising model phase diagram for many values of  $\alpha$ . The percolations threshold are 0.740 and 0.592 for  $\alpha = 0$  and  $0 < \alpha \leq 1$ , respectively. The dashed lines are only a guide to the eye.

$L$	$N_s$	$N_i$
50	20 – 150	3000 – 5000
100	05 – 50	3000 – 5000
150	05 – 50	3000 – 5000
300	05 – 50	3000 – 10000

Table 1

**Figure 1**

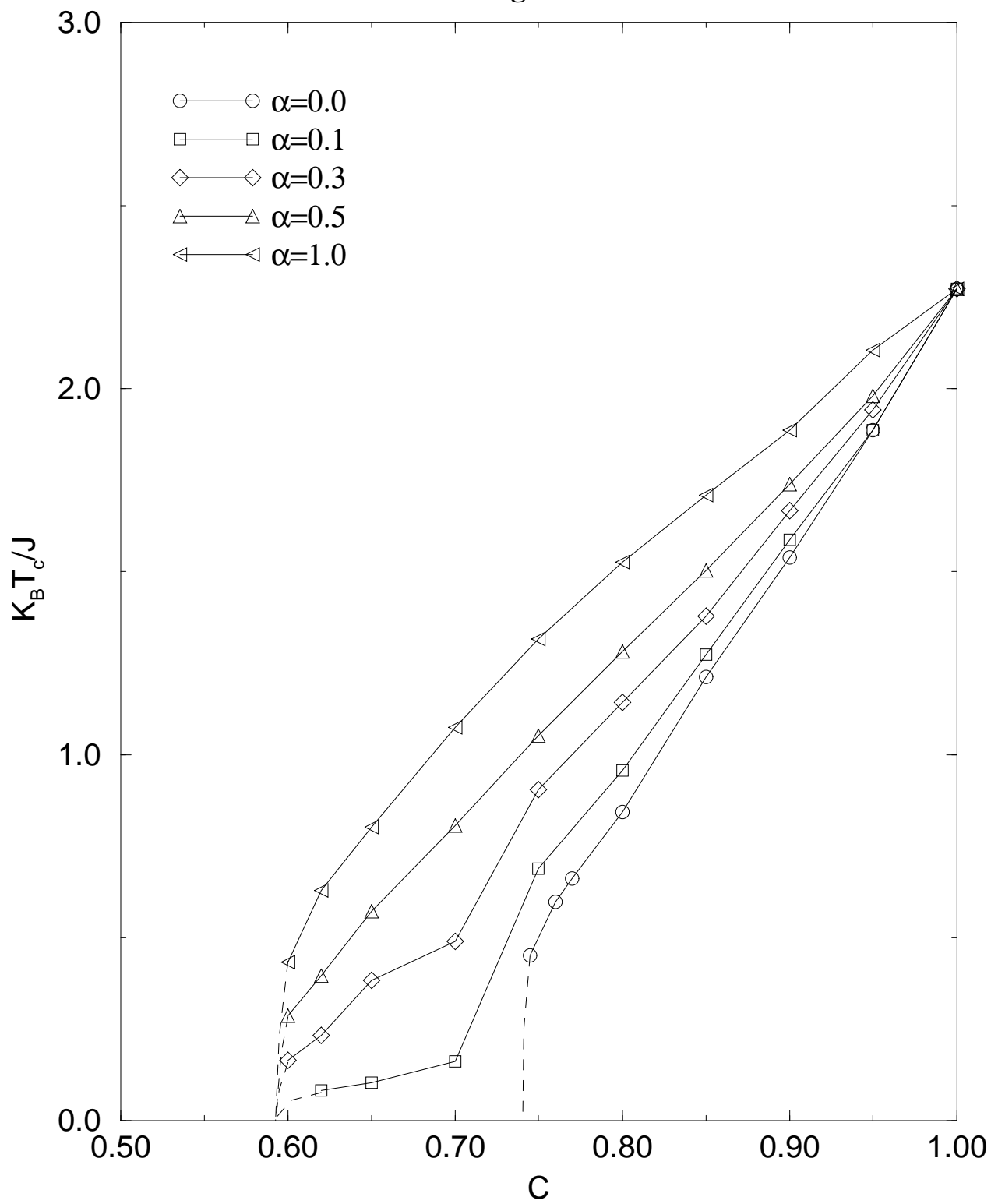


Figure 2

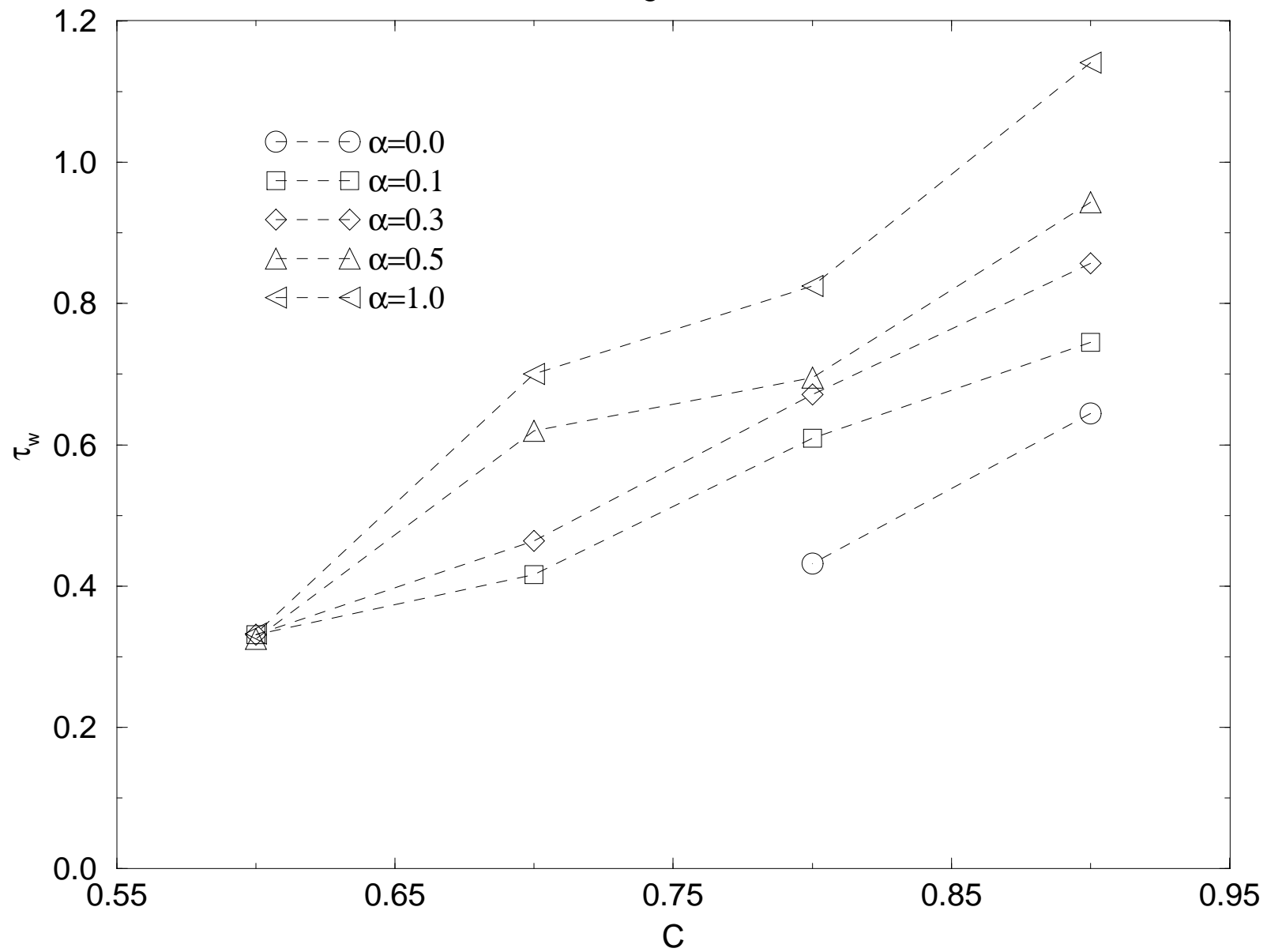




Figure 3

